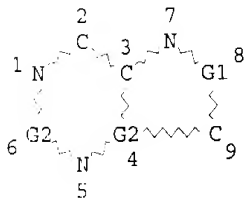
Structure 3a

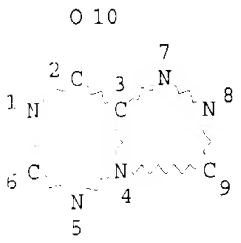
```
=> fil reg
FILE 'REGISTRY' ENTERED AT 14:25:00 ON 16 SEP 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   15 SEP 2002  HIGHEST RN 451445-11-7
DICTIONARY FILE UPDATES:  15 SEP 2002  HIGHEST RN 451445-11-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d his

     (FILE 'HCAPLUS' ENTERED AT 14:23:18 ON 16 SEP 2002)
               DEL  HIS Y

     FILE 'REGISTRY' ENTERED AT 14:23:35 ON 16 SEP 2002
               ACT THREEA/A
              ---------
L1                STR
L2   (       6184)SEA FILE=REGISTRY SSS FUL L1
L3   (        199)SEA FILE=REGISTRY ABB=ON  PLU=ON  333.885/RID
L4                STR
L5   (       6075)SEA FILE=REGISTRY SUB=L2 SSS FUL L1 NOT L4
L6   (         90)SEA FILE=REGISTRY ABB=ON  PLU=ON  L5 AND L3
L7                STR
L8             23 SEA FILE=REGISTRY SUB=L6 SSS FUL L7
               ---------

     FILE 'REGISTRY' ENTERED AT 14:25:00 ON 16 SEP 2002

=> d que stat l8
L1                STR
```




```
VAR G1=C/N/O/S
VAR G2=C/N
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
```

GRAPH ATTRIBUTES:
PSPEC I
NUMBER OF NODES IS 9

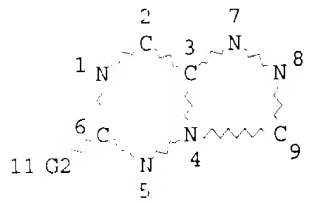
STEREO ATTRIBUTES: NONE
L2 (6184) SEA FILE=REGISTRY SSS FUL L1
L3 (199) SEA FILE=REGISTRY ABB=ON PLU=ON 333.885/RID
L4 STR

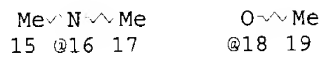


NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L5 (6075) SEA FILE=REGISTRY SUB=L2 SSS FUL L1 NOT L4
L6 (90) SEA FILE=REGISTRY ABB=ON PLU=ON L5 AND L3
L7 STR





VAR G2=H/NH2/16/13/F/CL/18/SH/OH/NO2/CF3/ME/ET/CN/22
NODE ATTRIBUTES:
CONNECT IS E3 RC AT 9
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 20

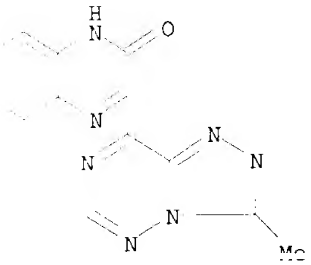
STEREO ATTRIBUTES: NONE
L8 23 SEA FILE=REGISTRY SUB=L6 SSS FUL L7

100.0% PROCESSED 90 ITERATIONS 23 ANSWERS

SEARCH TIME: 00.00.01

=> d ide can 18 23

L8 ANSWER 23 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 101073-86-3 REGISTRY
CN 2(1H)-Quinoxalinone, 3-(3-methyl-1,2,4-triazolo[3,4-f][1,2,4]triazin-8-yl)-
(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazine, 2(1H)-quinoxalinone deriv.
FS 3D CONCORD
MF C13 H9 N7 O
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

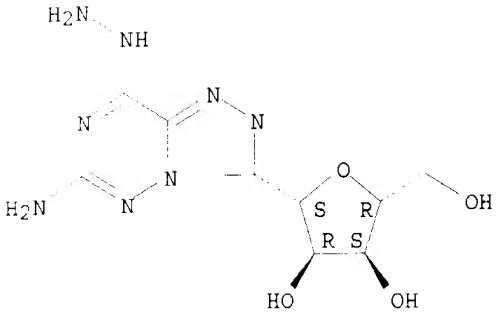
REFERENCE 1: 106:32982

REFERENCE 2: 104:129864

=> d ide can 18 1-23

L8 ANSWER 1 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 330469-95-9 REGISTRY
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazin-8(5H)-one, 6-amino-3-.beta.-D-
ribofuranosyl-, hydrazone (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C9 H14 N8 O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



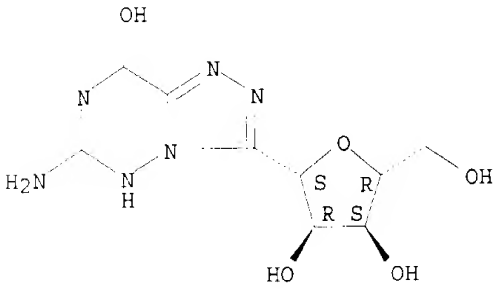
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:237749

L8 ANSWER 2 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 330469-94-8 REGISTRY
CN D-Ribitol, 1-C-(6-amino-5,8-dihydro-8-hydroxy-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C9 H14 N6 O5
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

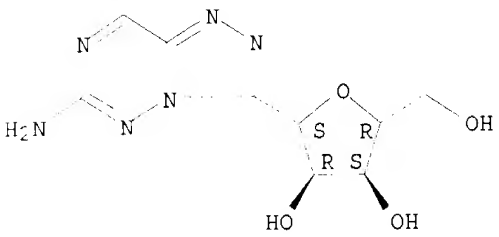
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:237749

L8 ANSWER 3 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 330469-93-7 REGISTRY
CN D-Ribitol, 1-C-(6-amino-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH

MF C9 H12 N6 O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



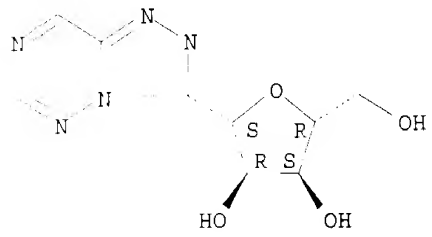
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:237749

L8 ANSWER 4 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 330469-92-6 REGISTRY
CN D-Ribitol, 1,4-anhydro-1-C-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl-, (1S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C9 H11 N5 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

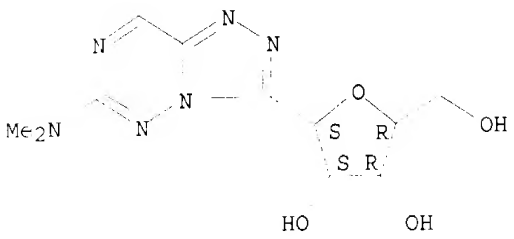
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:237749

L8 ANSWER 5 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 291536-68-0 REGISTRY
CN D-Arabinitol, 2,5-anhydro-5-C-[6-(dimethylamino)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, (5S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH

MF C11 H16 N6 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



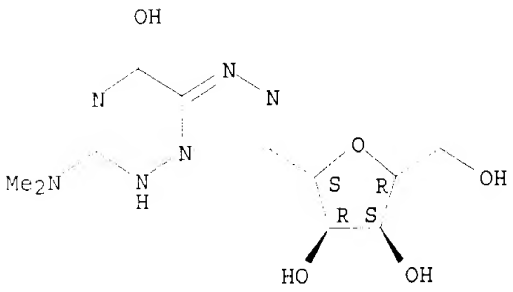
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:222974

L8 ANSWER 6 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 254440-96-5 REGISTRY
CN D-Ribitol, 1,4-anhydro-1-C-[6-(dimethylamino)-5,8-dihydro-8-hydroxy-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, (1S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H18 N6 O5
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

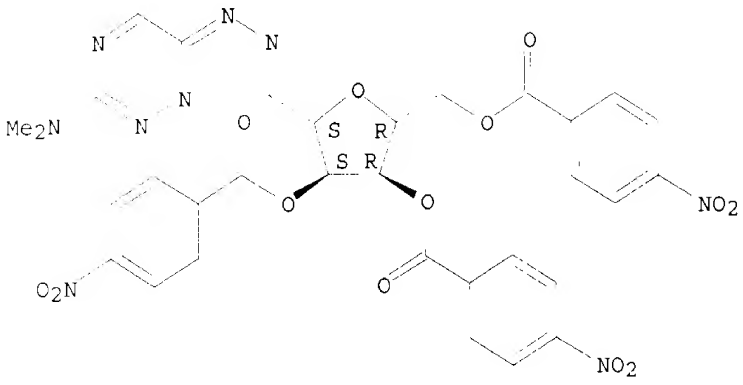
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 132:89887

L8 ANSWER 7 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 254440-95-4 REGISTRY
CN D-Ribitol, 1,4-anhydro-1-C-[6-(dimethylamino)-1,2,4-triazolo[3,4-

f][1,2,4]triazin-3-yl]-, 2,3,5-tris(4-nitrobenzoate), (1S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C32 H25 N9 O13
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



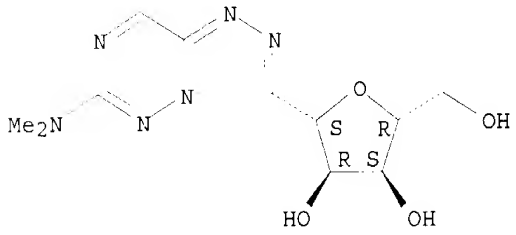
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 132:89887

L8 ANSWER 8 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 254440-94-3 REGISTRY
CN D-Ribitol, 1,4-anhydro-1-C-[6-(dimethylamino)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, (1S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H16 N6 O4
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

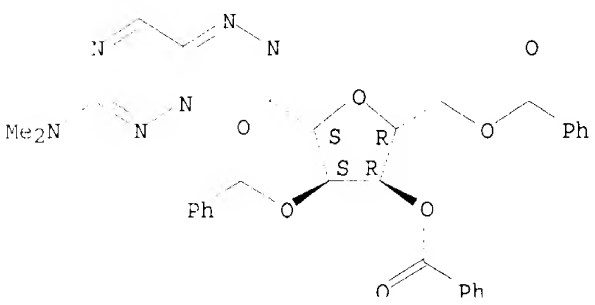
REFERENCE 1 134:237749

REFERENCE 2 133:222974

REFERENCE 3 132:89887

L8 ANSWER 9 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 254440-93-2 REGISTRY
CN D-Ribitol, 1,4-anhydro-1-C-[6-(dimethylamino)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, 2,3,5-tribenzoate, (1S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C32 H28 N6 O7
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

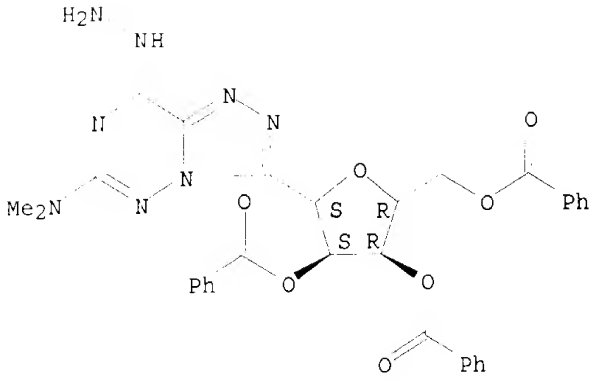
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1 133:222974

REFERENCE 2 132:89887

L8 ANSWER 10 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 254440-92-1 REGISTRY
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazin-8(5H)-one, 6-(dimethylamino)-3-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-, hydrazone (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C32 H30 N8 O7
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

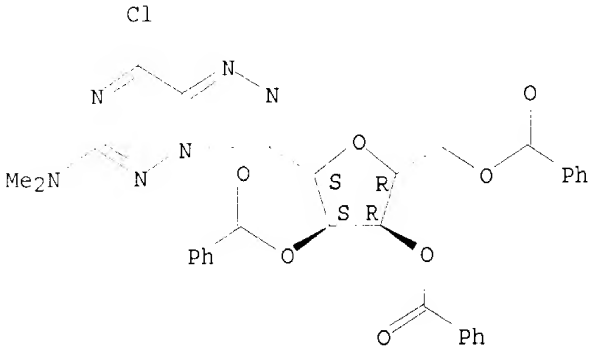
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:222974

REFERENCE 2: 132:89887

L8 ANSWER 11 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 254440-91-0 REGISTRY
CN D-Ribitol, 1,4-anhydro-1-C-[8-chloro-6-(dimethylamino)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, 2,3,5-tribenzoate, (1S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C32 H27 Cl N6 O7
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

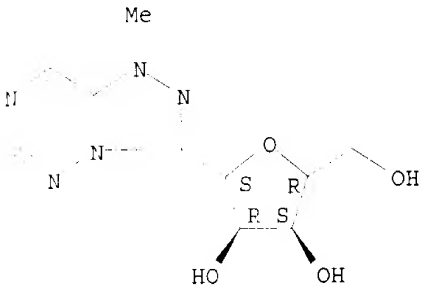
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:222974

REFERENCE 2: 132:89887

L8 ANSWER 12 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 143664-00-0 REGISTRY
CN D-Ribitol, 1,4-anhydro-1-C-(1,8a-dihydro-1-methyl-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl)-, (1S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazine, D-ribitol deriv.
FS STEREOSEARCH
MF C10 H15 N5 O4
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



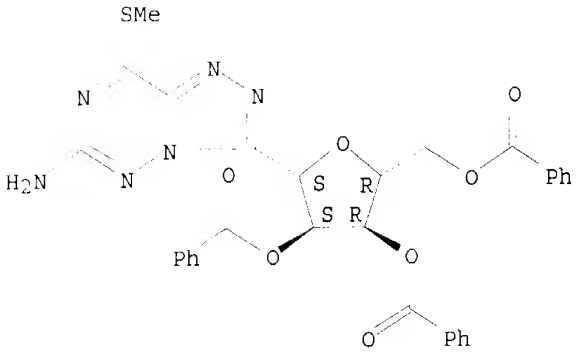
PROPEPTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1 117:192224

L8 ANSWER 13 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 103980-83-2 REGISTRY
CN D-Ribitol, 1-C-[6-amino-8-(methylthio)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-1,4-anhydro-, 2,3,5-tribenzoate, (1S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazine, D-ribitol deriv.
CN D-Ribitol, 1-C-[6-amino-8-(methylthio)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-1,4-anhydro-, 2,3,5-tribenzoate, (S)-
FS STEREOSEARCH
MF C31 H26 N6 O7 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

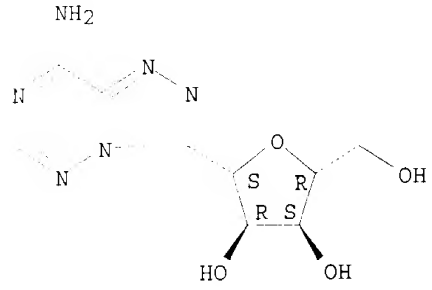
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:237749

REFERENCE 2: 105:172963

L8 ANSWER 14 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 103959-89-3 REGISTRY
CN D-Ribitol, 1-C-(8-amino-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl)-1,4-anhydro-, (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazine, D-ribitol deriv.
FS STEREOSEARCH
MF C9 H12 N6 O4
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



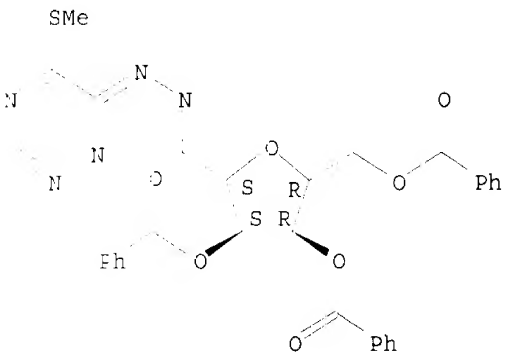
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 105:172963

L8 ANSWER 15 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 103959-88-2 REGISTRY
CN D-Ribitol, 1,4-anhydro-1-C-[8-(methylthio)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, 2,3,5-tribenzoate, (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazine, D-ribitol deriv.
FS STEREOSEARCH
MF C31 H25 N5 O7 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



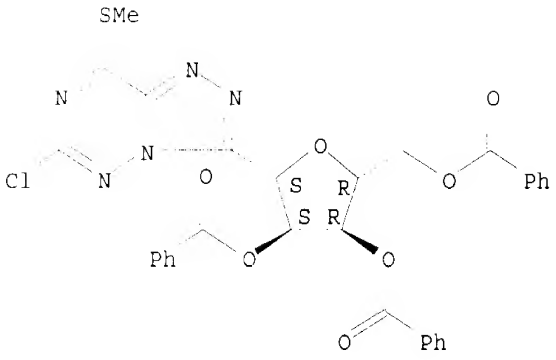
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1 105:172963

L8 ANSWER 16 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 103959-87-1 REGISTRY
CN D-Ribitol, 1,4-anhydro-1-C-[6-chloro-8-(methylthio)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, 2,3,5-tribenzoate, (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazine, D-ribitol deriv.
FS STEREOSEARCH
MF C31 H24 Cl N5 O7 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



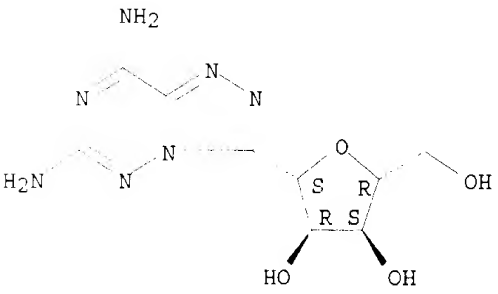
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 105:172963

L8 ANSWER 17 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 103959-86-0 REGISTRY
CN D-Ribitol, 1,4-anhydro-1-C-(6,8-diamino-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl)-, (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazine, D-ribitol deriv.
FS STEREOSEARCH
MF C9 H13 N7 O4
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

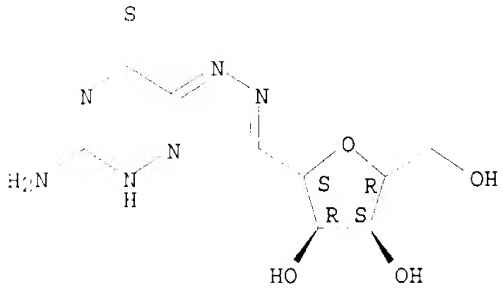
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 105:172963

L8 ANSWER 18 OF 23 REGISTRY COPYRIGHT 2002 ACS

RN 103959-85-9 REGISTRY
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazine-8(5H)-thione, 6-amino-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C9 H12 N6 O4 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



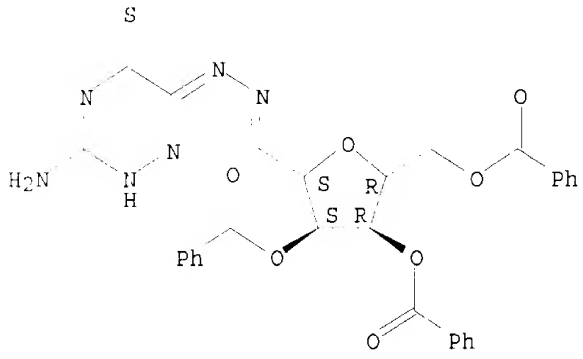
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 105:172963

L8 ANSWER 19 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 103959-84-8 REGISTRY
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazine-8(5H)-thione, 6-amino-3-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H24 N6 O7 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.

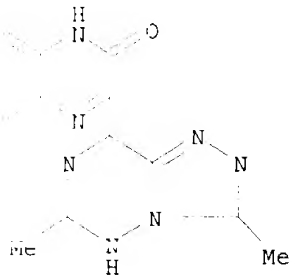


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 105:172963

L8 ANSWER 20 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 101129-12-8 REGISTRY
CN 2(1H)-Quinoxalinone, 3-(5,8-dihydro-3,6-dimethyl-1,2,4-triazolo[3,4-f][1,2,4]triazin-8-yl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazine, 2(1H)-quinoxalinone deriv.
FS 3D CONCORD
MF C14 H13 N7 O
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)



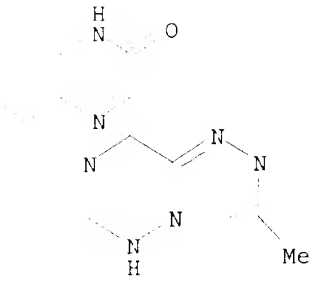
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 106:32982

REFERENCE 2: 104:129864

L8 ANSWER 21 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 101073-88-5 REGISTRY
CN 2(1H)-Quinoxalinone, 3-(5,8-dihydro-3-methyl-1,2,4-triazolo[3,4-f][1,2,4]triazin-8-yl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazine, 2(1H)-quinoxalinone deriv.
FS 3D CONCORD
MF C13 H11 N7 O
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)



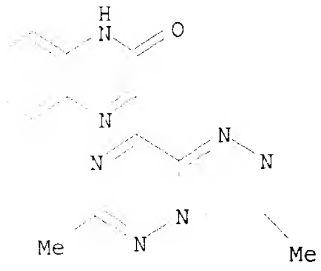
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 106:32982

REFERENCE 2: 104:129864

L8 ANSWER 22 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 101073-87-4 REGISTRY
CN 2(1H)-Quinoxalinone, 3-(3,6-dimethyl-1,2,4-triazolo[3,4-f][1,2,4]triazin-8-yl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazine, 2(1H)-quinoxalinone deriv.
FS 3D CONCORD
MF C14 H11 N7 O
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

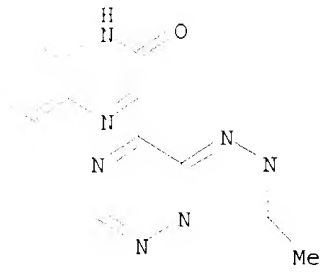
2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 106:32982

REFERENCE 2: 104:129864

L8 ANSWER 23 OF 23 REGISTRY COPYRIGHT 2002 ACS
RN 101073-86-3 REGISTRY

CN 2(1H)-Quinoxalinone, 3-(3-methyl-1,2,4-triazolo[3,4-f][1,2,4]triazin-8-yl)-
(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazine, 2(1H)-quinoxalinone deriv.
FS 3D CONCORD
MF C13 H9 N7 O
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 106:32982

REFERENCE 2: 104:129864

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 14:28:21 ON 16 SEP 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 16 Sep 2002 VOL 137 ISS 12
FILE LAST UPDATED: 15 Sep 2002 (20020915/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

CAS roles have been modified effective December 16, 2001. Please
check your SDI profiles to see if they need to be revised. For
information on CAS roles, enter HELP ROLES at an arrow prompt or use

=> d his l9

(FILE 'REGISTRY' ENTERED AT 10:51:05 ON 19 SEP 2002)

FILE 'HCAPLUS' ENTERED AT 10:51:14 ON 19 SEP 2002
L9 7 S L8

=> d .ca hitstr l9 1-7

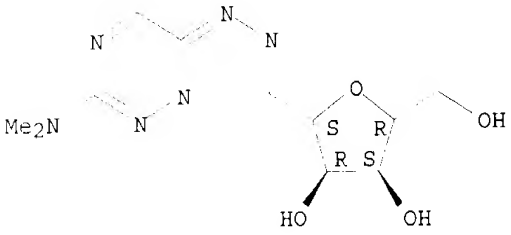
L9 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:139773 HCAPLUS
DOCUMENT NUMBER 134:237749
TITLE: Design and Synthesis of Inhibitors of Adenosine and AMP Deaminases
AUTHOR(S): Bojack, Guido; Earnshaw, Christopher G.; Klein, Robert; Lindell, Stephen D.; Lowinski, Christian; Preuss, Rainer
CORPORATE SOURCE: Aventis CropScience GmbH, Frankfurt am Main, D-65926, Germany
SOURCE: Organic Letters (2001), 3(6), 839-842
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE English
AB Nucleosides and nucleotides which are able to undergo covalent hydration in the aglycon ring system are potential inhibitors of the enzymes adenosine deaminase (ADA) and AMP deaminase, resp. Calcns. of the enthalpy of covalent hydration and of enzyme binding energy have been used to design new inhibitors of ADA. The ribosyl triazolotriazine I, which was synthesized as a result of these calcns., exists predominantly as the covalent hydrate II in water and is a potent inhibitor of mammalian ADA (IC50 50 nM). In addn., biol. testing of the I/II mixt. showed that it possessed postemergence herbicidal activity at rates of 320 g ha-1 and below, depending upon the species.
CC 33-9 (Carbohydrates)
Section cross-reference(s): 5, 7
IT 550-33-4, Nebularine 13264-01-2, Deaminoformycin 206450-52-4
254114-35-7 **254440-94-3** 291536-67-9 330469-91-5
330469-92-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(design and synthesis of C-nucleoside based inhibitors of adenosine and AMP deaminases)
IT **330469-93-7P 330469-94-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(design and synthesis of C-nucleoside based inhibitors of adenosine and AMP deaminases)
IT **103980-83-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(design and synthesis of C-nucleoside based inhibitors of adenosine and AMP deaminases)
IT **330469-95-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(design and synthesis of C-nucleoside based inhibitors of adenosine and

AMP deaminases)

IT **254440-94-3 330469-92-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(design and synthesis of C-nucleoside based inhibitors of adenosine and AMP deaminases)

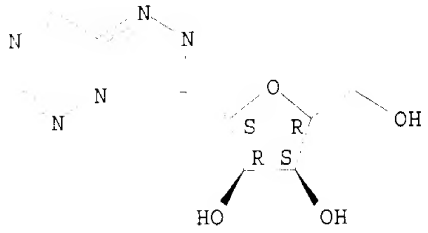
RN 254440-94-3 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-[6-(dimethylamino)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 330469-92-6 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl-, (1S)- (9CI) (CA INDEX NAME)

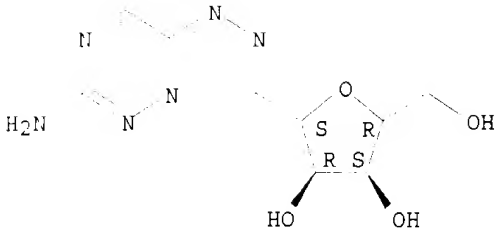
Absolute stereochemistry.



IT **330469-93-7P 330469-94-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(design and synthesis of C-nucleoside based inhibitors of adenosine and AMP deaminases)

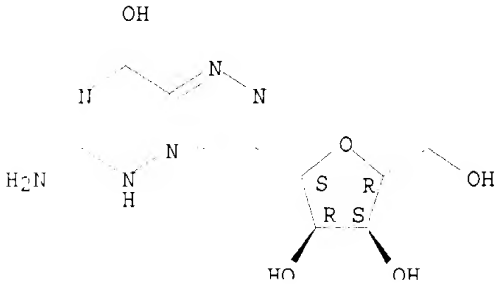
RN 330469-93-7 HCAPLUS
CN D-Ribitol, 1-C-(6-amino-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



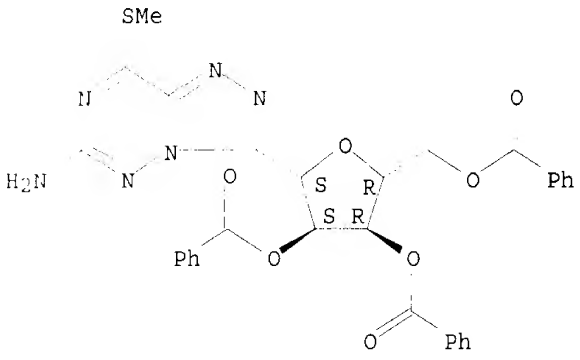
RN 330469-94-8 HCAPLUS
CN D-Ribitol, 1-C-(6-amino-5,8-dihydro-8-hydroxy-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl)-1,4-anhydro-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **103980-83-2**
PL: RCT (Reactant); RACT (Reactant or reagent)
(design and synthesis of C-nucleoside based inhibitors of adenosine and AMP deaminases)
RN 103980-83-2 HCAPLUS
CN D-Ribitol, 1-C-[6-amino-8-(methylthio)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-1,4-anhydro-, 2,3,5-tribenzoate, (1S)- (9CI) (CA INDEX NAME)

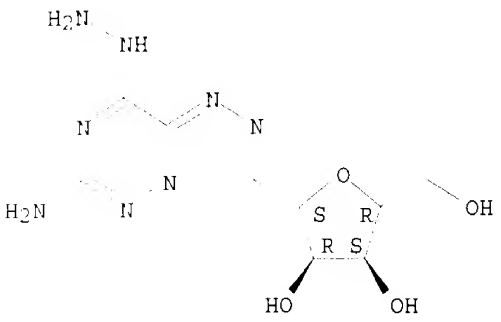
Absolute stereochemistry.



IT **330469-95-9P**
PL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(design and synthesis of C-nucleoside based inhibitors of adenosine and

AMP deaminases)
RN 330469-95-9 HCAPLUS
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazin-8(5H)-one, 6-amino-3-.beta.-D-ribofuranosyl-, hydrazone (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:665549 HCAPLUS
DOCUMENT NUMBER: 133:222974
TITLE: Preparation of C-nucleosides as adenosine monophosphate deaminase regulators for use in agriculture or medicine
INVENTOR(S): Bojack, Guido; Lindell, Stephen; Rosinger, Christopher; Dudfield, Philip; Earnshaw, Christopher
PATENT ASSIGNEE(S): Aventis Cropscience Gmbh, Germany
SOURCE: Ger. Offen., 82 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19912636	A1	20000921	DE 1999-19912636	19990320
WO 2000056734	A1	20000928	WO 2000-EP2206	20000313
W: AE, AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1165563	A1	20020102	EP 2000-916932	20000313
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

PRIORITY APPLN. INFO.: DE 1999-19912636 A 19990320
WO 2000-EP2206 W 20000313

OTHER SOURCE(S): MARPAT 133:222974
AB Title compds. [(I); Q = N, CR1; Q1 = C,N; if Q1 = C, bond Q1-C2 = double; if Q1 = N, bond C2-Q2 = double; Q2 = N, CR2, when Q1 = N, or NR2, O, S,

S(O), SO2, when Q1 = C; R = (un)satd. hydrocarbon chain substituted with O, S, NHR4; R1, R2 independently = H, NHR3, OR3, SR3, CN, halogen, N3, NO2, SF5; R3 = H, acyl, (un)satd. (cyclo)alkyl, SO2NH2; R4 = alkyl], useful as herbicides, plant growth regulators, and for the treatment of disease as adenosine monophosphate deaminase or adenosine deaminase regulators, were prepd. Thus, in four steps, starting from 2',3',5'-tri-O-acetyl-8-aza-9-deaza-inosine, (II) was prepd. (isolated as the disodium salt). In in vitro adenosine monophosphate deaminase regulation tests in pea plants or calf intestine, II had .gtoreq. 50% inhibition of enzyme activity at 500.mu.M. Similar compds. were tested for activity with adenosine deaminase from rabbit muscle, and also proved active.

IC ICM C07H007-06
ICS C07H023-00; C07H009-04; C07H015-26; C07D487-04; C07D519-00; A01N043-90; A01N057-16; A01N055-10; A61K031-66; A61K031-695; A61K031-70

CC 33-9 (Carbohydrates)
Section cross-reference(s): 5, 28, 63

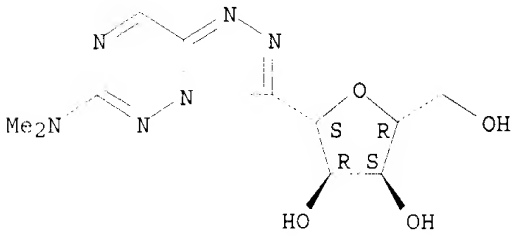
IT 244035-94-7P 254114-35-7P **254440-94-3P** 291536-67-9P **291536-68-0P** 291536-69-1P 291536-70-4P 291536-71-5P 291536-72-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn of C-nucleosides as adenosine monophosphate deaminase regulators for use in agriculture or medicine)

IT 13264-01-2P 33822-98-9P 54317-66-7P 254114-42-6P 254114-43-7P 254114-44-8P 254114-51-7P 254440-83-0P 254440-87-4P 254440-88-5P 254440-89-6P **254440-91-0P 254440-92-1P** **254440-93-2P** 291536-61-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn of C-nucleosides as adenosine monophosphate deaminase regulators for use in agriculture or medicine)

IT **254440-94-3P 291536-68-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn of C-nucleosides as adenosine monophosphate deaminase regulators for use in agriculture or medicine)

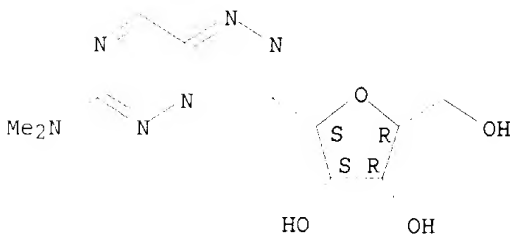
RN 254440-94-3 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-[6-(dimethylamino)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 291536-68-0 HCAPLUS
CN D-Arabinitol, 2,5-anhydro-5-C-[6-(dimethylamino)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

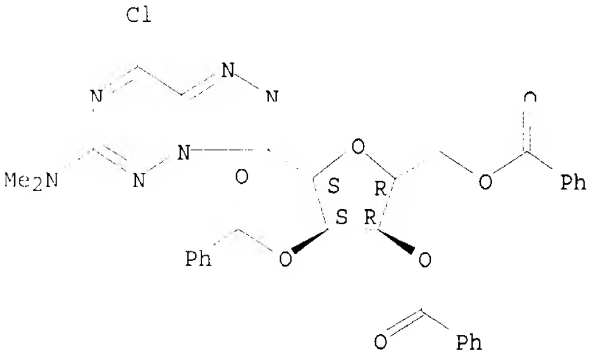


IT **254440-91-0P 254440-92-1P 254440-93-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of C-nucleosides as adenosine monophosphate deaminase regulators for use in agriculture or medicine)

RN 254440-91-0 HCAPLUS

CN D-Ribitol, 1,4-anhydro-1-C-[8-chloro-6-(dimethylamino)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, 2,3,5-tribenzoate, (1S)- (9CI) (CA INDEX NAME)

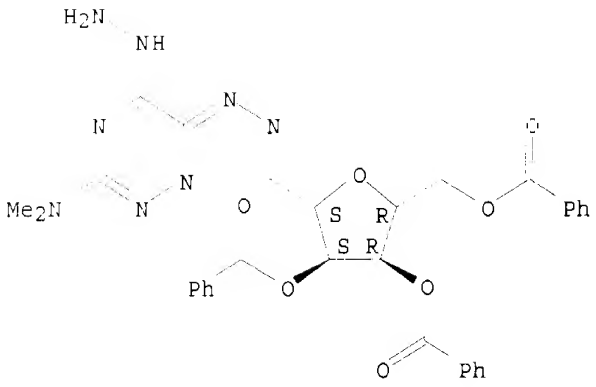
Absolute stereochemistry.



RN 254440-92-1 HCAPLUS

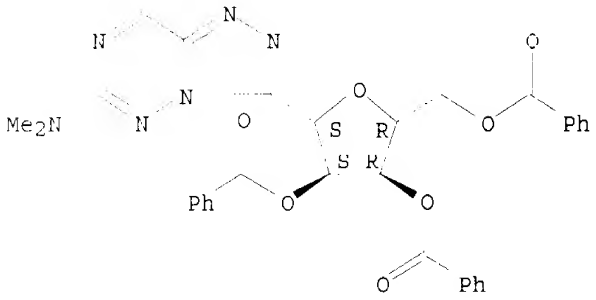
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazin-8(5H)-one, 6-(dimethylamino)-3-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-, hydrazone (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 254440-93-2 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-[6-(dimethylamino)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, 2,3,5-tribenzoate, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:669962 HCAPLUS
DOCUMENT NUMBER: 132:89887
TITLE: Synthesis of C-ribosyl 1,2,4-triazolo[3,4-f][1,2,4]triazines as inhibitors of adenosine and AMP deaminases
AUTHOR(S): Dudfield, Philip J.; Le, Van-Duc; Lindell, Stephen D.; Rees, Charles W.
CORPORATE SOURCE: AgrEvo UK Limited, Saffron Walden, CB10 1XL, UK
SOURCE Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (20), 2937-2942
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:89887
AB Modified C-nucleosides and nucleotides with an enhanced tendency to undergo covalent hydration are of interest as potential inhibitors of adenosine deaminase (ADA) and AMP deaminase, resp. In a search for such compds. we have synthesized 6-dimethylamino-3-(.beta.-D-ribofuranosyl)-1,2,4-triazolo[3,4-f][1,2,4]triazine 4 in four steps (42% overall yield) from the readily available allonic acid 6 and the hydrazine 7. The

hydrazide 16 derived from 6 and 7 (78%) is converted directly into the cyclized chloro compd. 19 (62%) with phosphorus trichloride oxide, followed by dechlorination (96%) and deprotection (90%). Riboside 4 undergoes partial hydration in water to the covalent hydrate 22, and is a modest inhibitor of mammalian ADA (IC50 180 .mu.M).

CC 7-3 (Enzymes)
Section cross-reference(s): 33

IT **254440-94-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn of C-ribosyl 1,2,4-triazolo[3,4-f][1,2,4]triazines as inhibitors of adenosine and AMP deaminases)

IT **254440-96-5P**
RL: BYP (Byproduct); PREP (Preparation)
(prepn of C-ribosyl 1,2,4-triazolo[3,4-f][1,2,4]triazines as inhibitors of adenosine and AMP deaminases)

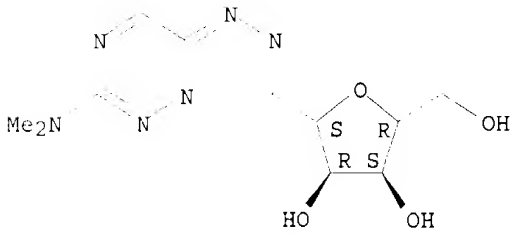
IT 23316-67-8P 23316-68-9P 53300-17-7P 54317-48-5P 54317-66-7P 63197-14-8P 254440-83-0P 254440-84-1P 254440-85-2P 254440-87-4P 254440-88-5P 254440-89-6P **254440-91-0P 254440-92-1P 254440-93-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn of C-ribosyl 1,2,4-triazolo[3,4-f][1,2,4]triazines as inhibitors of adenosine and AMP deaminases)

IT 254440-90-9P **254440-95-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn of C-ribosyl 1,2,4-triazolo[3,4-f][1,2,4]triazines as inhibitors of adenosine and AMP deaminases)

IT **254440-94-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn of C-ribosyl 1,2,4-triazolo[3,4-f][1,2,4]triazines as inhibitors of adenosine and AMP deaminases)

RN 254440-94-3 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-[6-(dimethylamino)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, (1S)- (9CI) (CA INDEX NAME)

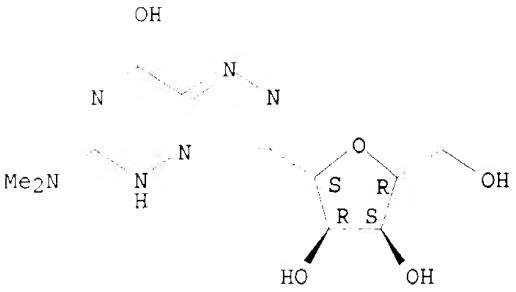
Absolute stereochemistry.



IT **254440-96-5P**
RL: BYP (Byproduct); PREP (Preparation)
(prepn of C-ribosyl 1,2,4-triazolo[3,4-f][1,2,4]triazines as inhibitors of adenosine and AMP deaminases)

RN 254440-96-5 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-[6-(dimethylamino)-5,8-dihydro-8-hydroxy-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

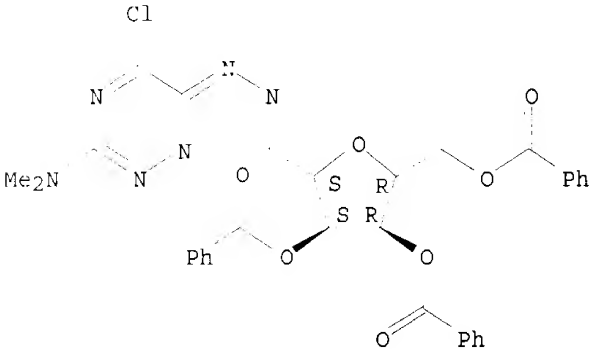


IT **254440-91-0P 254440-92-1P 254440-93-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation), RACT (Reactant or reagent)
(prepn. of C-ribosyl 1,2,4-triazolo[3,4-f][1,2,4]triazines as inhibitors of adenosine and AMP deaminases)

RN 254440-91-0 HCAPLUS

CN D-Ribitol, 1,4-anhydro-1-C-[8-chloro-6-(dimethylamino)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, 2,3,5-tribenzoate, (1S)- (9CI) (CA INDEX NAME)

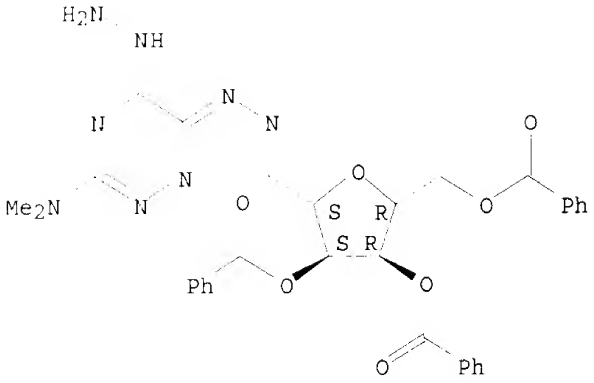
Absolute stereochemistry.



RN 254440-92-1 HCAPLUS

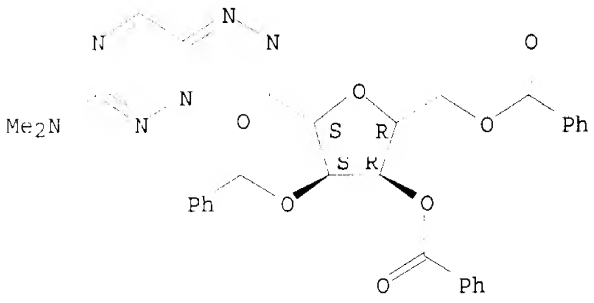
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazin-8(5H)-one, 6-(dimethylamino)-3-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-, hydrazone (9CI) (CA INDEX NAME)

Absolute stereochemistry.



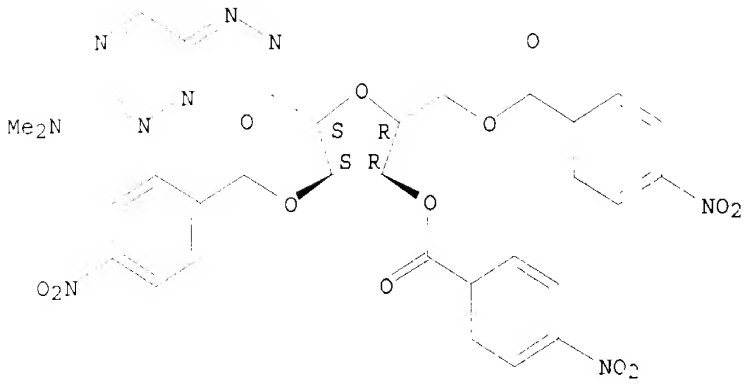
RN 254440-93-2 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-[6-(dimethylamino)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, 2,3,5-tribenzoate, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **254440-95-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of C-ribosyl 1,2,4-triazolo[3,4-f][1,2,4]triazines as inhibitors of adenosine and AMP deaminases)
RN 254440-95-4 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-[6-(dimethylamino)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, 2,3,5-tris(4-nitrobenzoate), (1S)- (9CI) (CA INDEX NAME)

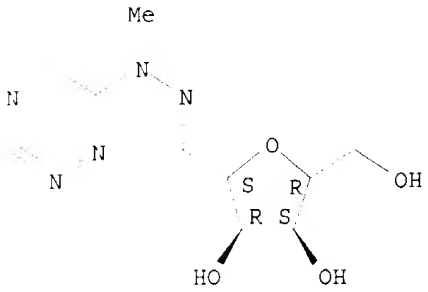
Absolute stereochemistry.



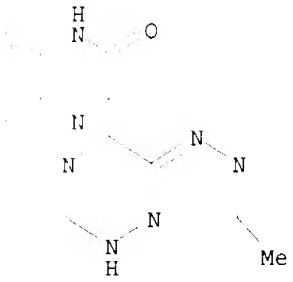
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1992:592224 HCAPLUS
DOCUMENT NUMBER: 117:192224
TITLE: Use of distance geometry approach for the in vitro antiviral activity evaluation of N-bridgehead C-nucleosides
AUTHOR(S): Kobe, B.; Kobe, J.; Smee, D. F.; Jerman-Blazic-Dzonova, B.; Solmajer, T.
CORPORATE SOURCE: Dep. Chem., Univ. Ljubljana, Ljubljana, 61000, Yugoslavia
SOURCE: Eur. J. Med. Chem. (1992), 27(3), 259-66
CODEN: EJMCA5; ISSN: 0223-5234
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A 3-dimensional receptor model of parainfluenza virus type 3 developed by Chose et al using the distance geometry approach to analyze the in vitro antiviral activity of several novel ribonucleosides from imidazotriazine, imidazo-pyrazine and triazolo-pyrazine and pyridine series, have been used. On the basis of at. physicochem. properties ie hydrophobicity, molar refractivity and charge d. the interaction energy of min. energy conformations of 22 compds. with hypothetic virus active site were evaluated. Seven nucleosides from imidazopyrazine and imidazotriazine series have shown significantly high calcd values of virus rating while the analogs with triazolopyrazine, triazolopyridine and pyrazolo-pyridine heterocycles are expected to have only slight or moderate virus activity.
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 22
IT 342-69-8 13877-76-4 41329-11-7 67410-65-5 68797-10-4 68797-11-5 68797-12-6 103959-90-6 104885-87-2 104885-95-2 142588-97-4 143663-90-5 143663-91-6 143663-92-7 143663-93-8 143663-94-9 143663-95-0 143663-96-1 143663-97-2 143663-98-3 143663-99-4 **143664-00-0** 143989-88-2
RL: RCT (Reactant)
(conformation and MSBAR virus rating of)
IT **143664-00-0**
RL: RCT (Reactant)
(conformation and MSBAR virus rating of)
RN 143664-00-0 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-(1,8a-dihydro-1-methyl-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl)-, (1S)- (9CI) (CA INDEX NAME)

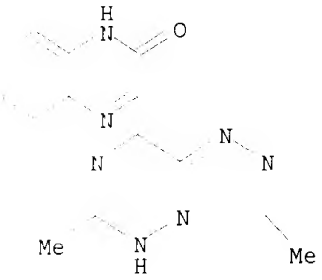
Absolute stereochemistry.



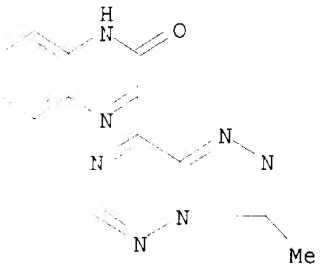
L9 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1987:32982 HCAPLUS
DOCUMENT NUMBER: 106:32982
TITLE: Synthesis and conversions of 3-(4-amino-5-methyl-4H-1,2,4-triazol-3-ylmethylene)-2-oxo-1,2,3,4-tetrahydroquinoxaline
AUTHOR(S): Kurasawa, Yoshihisa; Okamoto, Yoshihisa; Takada, Atsushi
CORPORATE SOURCE: Sch. Pharm. Sci., Kitasato Univ., Tokyo, 108, Japan
SOURCE: J. Heterocycl. Chem. (1985), 22(6), 1715-18
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 106:32982
AB Reaction of hydrazone I with N2H4 in DBU-EtOH gave 3-(4-amino-5-methyl-4H-1,2,4-triazol-3-ylmethylene)-2-oxo-1,2,3,4-tetrahydroquinoxaline, whose reactions with an equimolar and 2-fold molar amt. of HNO2 afforded hydroxyiminotriazolylmethylquinoxalines II and III. II and II were converted to cyclic compds.
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
IT **101073-88-5P 101129-12-8P**
RL RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and oxidn. of)
IT 96409-37-9P 96409-38-0P 96409-41-5P 96409-42-6P 96409-43-7P
96409-44-8P 96409-45-9P **101073-86-3P 101073-87-4P**
RL SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **101073-88-5P 101129-12-8P**
RL RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and oxidn. of)
RN 101073-88-5 HCAPLUS
CN 2(1H)-Quinoxalinone, 3-(5,8-dihydro-3-methyl-1,2,4-triazolo[3,4-f][1,2,4]triazin-8-yl)- (9CI) (CA INDEX NAME)



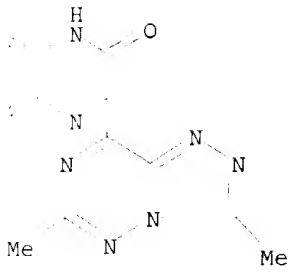
RN 101129-12-8 HCAPLUS
CN 2(1H)-Quinoxalinone, 3-(5,8-dihydro-3,6-dimethyl-1,2,4-triazolo[3,4-f][1,2,4]triazin-8-yl)- (9CI) (CA INDEX NAME)



IT **101073-86-3P 101073-87-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 101073-86-3 HCAPLUS
CN 2(1H)-Quinoxalinone, 3-(3-methyl-1,2,4-triazolo[3,4-f][1,2,4]triazin-8-yl)- (9CI) (CA INDEX NAME)



RN 101073-87-4 HCAPLUS
CN 2(1H)-Quinoxalinone, 3-(3,6-dimethyl-1,2,4-triazolo[3,4-f][1,2,4]triazin-8-yl)- (9CI) (CA INDEX NAME)

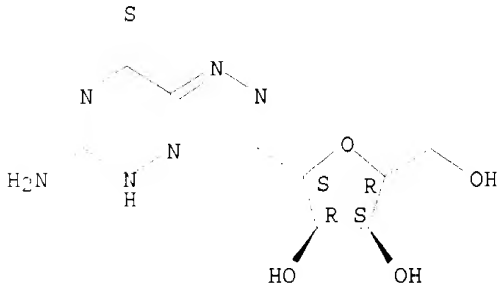


L9 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:572963 HCAPLUS
DOCUMENT NUMBER: 105:172963
TITLE: Synthesis and antitumor activity of certain 3-.beta.-D-ribofuranosyl-1,2,4-triazolo[3,4-f]-1,2,4-triazines related to formycin prepared via ring closure of a 1,2,4-triazine precursor
AUTHOR(S): Ramasamy, Kandasamy; Ugarkar, Bheemarao G.; McKernan, Patricia A.; Robins, Roland K.; Revankar, Ganapathi R.
CORPORATE SOURCE: Cancer Res. Cent., Brigham Young Univ., Provo, UT, 84602, USA
SOURCE: J. Med. Chem. (1986), 29(11), 2231-5
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:172963
AB Title C-nucleosides I [R = NH2, R1 = H (II); R = R1 = H] and III were prepd. from 3-amino-6-hydrazino-1,2,4-triazin-5(4H)-one (IV) and a 2,5-anhydroallonic acid deriv., and their antitumor activity was detd. Thus, dehydrative coupling of IV with 3,4,6-tri-O-benzoyl-2,5-anhydro-D-allonic acid and further ring closure of the product gave I (R = NH2, R1 = Bz), which on treatment with MeONa in MeOH gave II. III showed pronounced inhibiting effects against L1210, WIL2, and CCRF-CEM cell lines with ID50 values ranging from 5.0 to 7.3 .mu.M.
CC 23-9 (Carbohydrates)
Section cross-reference(s): 1, 28
IT 6742-12-7DP, ribofuranosyltriazolotriazines related to 103959-83-7P **103959-85-9P 103959-86-0P 103959-89-3P** 103959-90-6P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antitumor activity of)
IT **103959-84-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and debenzylation or methylation of)
IT **103959-88-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, with ammonia)
IT **103980-83-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reactions of)
IT **103959-87-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **103959-85-9P 103959-86-0P 103959-89-3P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic

preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antitumor activity of)

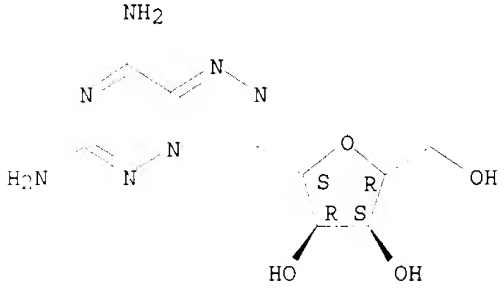
RN 103959-85-9 HCAPLUS
CN 1,2,4-Triazolo[3,4-f][1,2,4]triazine-8(5H)-thione, 6-amino-3-.beta.-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



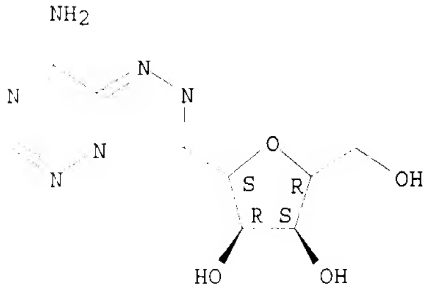
RN 103959-86-0 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-(6,8-diamino-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 103959-89-3 HCAPLUS
CN D-Ribitol, 1-C-(8-amino-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl)-1,4-anhydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



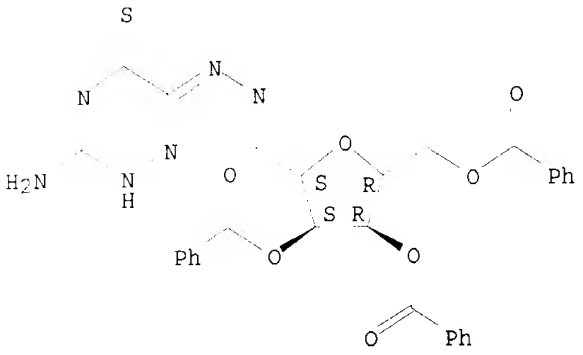
IT **103959-84-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and debenzylation or methylation of)

RN 103959-84-8 HCAPLUS

CN 1,2,4-Triazolo[3,4-f][1,2,4]triazine-8(5H)-thione, 6-amino-3-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



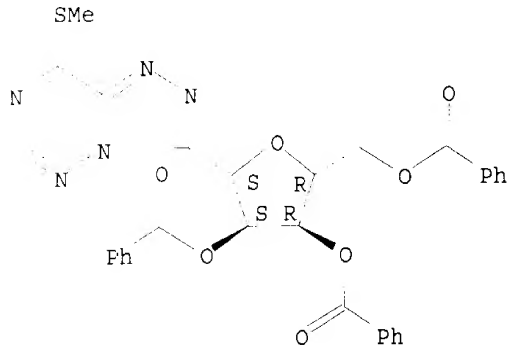
IT **103959-88-2P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, with ammonia)

RN 103959-88-2 HCAPLUS

CN D-Ribitol, 1,4-anhydro-1-C-[8-(methylthio)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, 2,3,5-tribenzoate, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



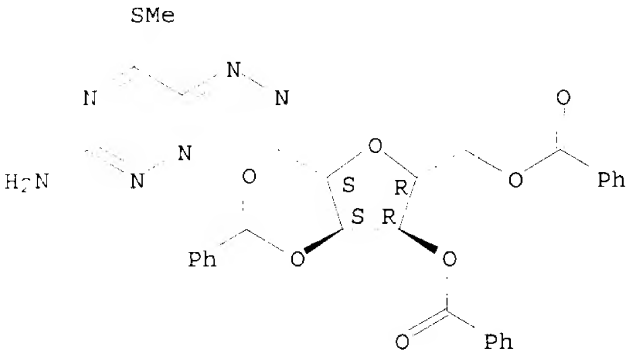
IT **103980-83-2P**

RL RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reactions of)

RN 103980-83-2 HCAPLUS

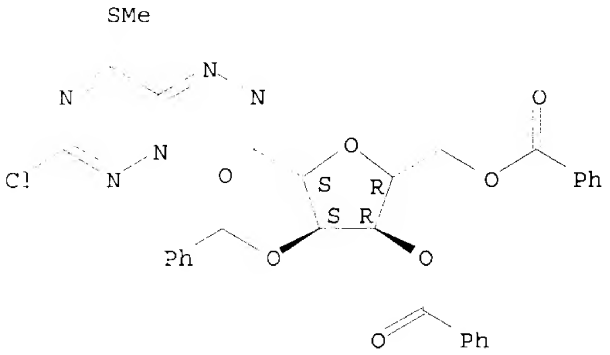
CN D-Ribitol, 1-C-[6-amino-8-(methylthio)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-1,4-anhydro-, 2,3,5-tribenzoate, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **103959-87-1P**
PL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 103959-87-1 HCAPLUS
CN D-Ribitol, 1,4-anhydro-1-C-[6-chloro-8-(methylthio)-1,2,4-triazolo[3,4-f][1,2,4]triazin-3-yl]-, 2,3,5-tribenzoate, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

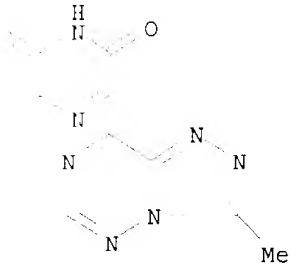


L9 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:129864 HCAPLUS
DOCUMENT NUMBER: 104:129864
TITLE A new method for the synthesis of novel 1,2,4-triazolo[3,4-f][1,2,4]triazines
AUTHOR(S): Kurasawa, Yoshihisa; Okamoto, Yoshihisa; Takada, Atsushi
CORPORATE SOURCE: Sch. Pharm. Sci., Kitasato Univ., Tokyo, 108, Japan
SOURCE: J. Heterocycl. Chem. (1985), 22(3), 935-6
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:129864
AB Treating the oxime I with ortho esters RC(OEt)3 (R = H, Me) in the presence of Fe powder in HOAc gave the title triazines II, as well as the dihydrotriazolotriazines III, which were readily oxidized to II.
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
IT **101073-86-3P 101073-87-4P 101073-88-5P**
101129-12-8P

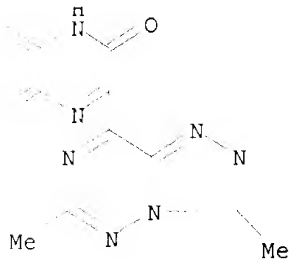
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **101073-86-3P 101073-87-4P 101073-88-5P**
101129-12-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

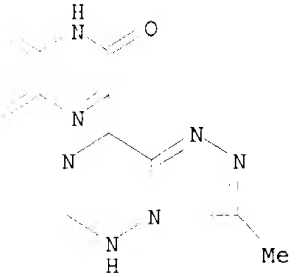
RN 101073-86-3 HCAPLUS
CN 2(1H)-Quinoxalinone, 3-(3-methyl-1,2,4-triazolo[3,4-f][1,2,4]triazin-8-yl)- (9CI) (CA INDEX NAME)



RN 101073-87-4 HCAPLUS
CN 2(1H)-Quinoxalinone, 3-(3,6-dimethyl-1,2,4-triazolo[3,4-f][1,2,4]triazin-8-yl)- (9CI) (CA INDEX NAME)



RN 101073-88-5 HCAPLUS
CN 2(1H)-Quinoxalinone, 3-(5,8-dihydro-3-methyl-1,2,4-triazolo[3,4-f][1,2,4]triazin-8-yl)- (9CI) (CA INDEX NAME)



RN 101129-12-8 HCAPLUS
CN 2(1H)-Quinoxalinone, 3-(5,8-dihydro-3,6-dimethyl-1,2,4-triazolo[3,4-f][1,2,4]triazin-8-yl)- (9CI) (CA INDEX NAME)